Scientific Computing & Modelling

References

ADF Program System
Release 2009.01

Scientific Computing & Modelling NV
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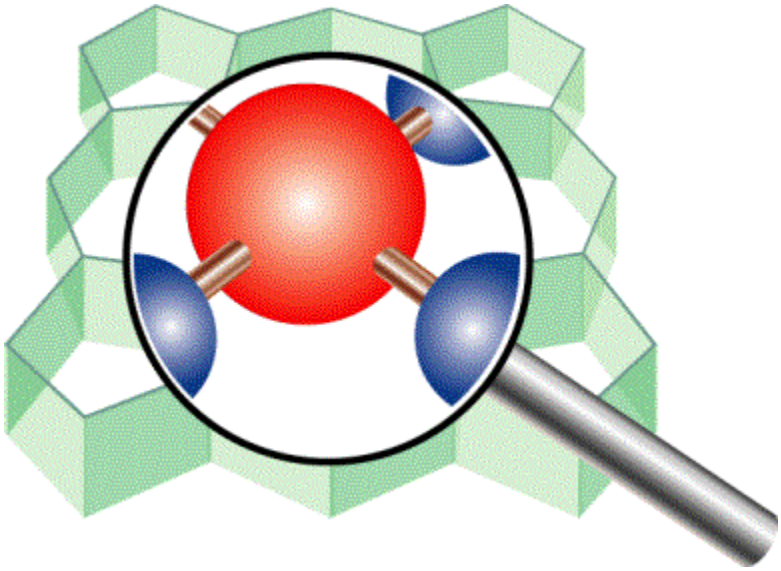

Table of Contents

General References

When you publish results in the scientific literature that were obtained with programs of the ADF package, you are required to include references to the program package with the appropriate release number, and a few key publications.

In addition to these general references, references to special features are mandatory, in case you have used them. See the section Feature References ADF and Feature References BAND.

ADF

For calculations with the molecular ADF program, version 2009.01:

1. G. te Velde, F.M. Bickelhaupt, S.J.A. van Gisbergen, C. Fonseca Guerra, E.J. Baerends, J.G. Snijders and T. Ziegler, *Chemistry with ADF.* Journal of Compututational Chemistry **22**, 931 (2001)

2. C. Fonseca Guerra, J.G. Snijders, G. te Velde and E.J. Baerends, *Towards an order-N DFT method.* Theoretical Chemistry Accounts **99**, 391 (1998)

3. ADF2009.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com
Optionally, you may add the following list of authors and contributors:
E.J. Baerends, J. Autschbach, D. Bashford, A. Bérces, F.M. Bickelhaupt, C. Bo, P.M. Boerrigter, L. Cavallo, D.P. Chong, L. Deng, R.M. Dickson, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, C. Fonseca Guerra, A. Ghysels, A. Giammona, S.J.A. van Gisbergen, A.W. Götz, J.A. Groeneveld, O.V. Gritsenko, M. Grüning, F.E. Harris, P. van den Hoek, C.R. Jacob, H. Jacobsen, L. Jensen, G. van Kessel, F. Kootstra, M.V. Krykunov, E. van Lenthe, D.A. McCormack, A. Michalak, M. Mitoraj, J. Neugebauer, V.P. Nicu, L. Noodleman, V.P. Osinga, S. Patchkovskii, P.H.T. Philipsen, D. Post, C.C. Pye, W. Ravenek, J.I. Rodríguez, P. Ros, P.R.T. Schipper, G. Schreckenbach, M. Seth, J.G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo, A.L. Yakovlev, and T. Ziegler

Note: if you have used a modified (by yourself, for instance) version of the code, you should mention in the citation that a modified version has been used.

BAND

For calculations with the periodic structures BAND program, version 2009.01:

1. G. te Velde and E.J. Baerends, *Precise density-functional method for periodic structures.* Physical Review B **44**, 7888 (1991)

2. G. Wiesenekker and E.J. Baerends, *Quadratic integration over the three-dimensional Brillouin zone.* Journal of Physics: Condensed Matter **3**, 6721 (1991)

3. BAND2009.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com
Optionally, you may add the following list of authors and contributors:
G. te Velde, E.J. Baerends, P.H.T. Philipsen, G. Wiesenekker, J.A. Groeneveld, J.A. Berger, P.L. de Boeij, R. Klooster, F. Kootstra, P. Romaniello, J.G. Snijders, E.S. Kadantsev, T. Ziegler

Note: if you have used a modified (by yourself, for instance) version of the code, you should mention in the citation that a modified version has been used.

COSMO-RS

For calculations with the COSMO-RS program, version 2009.01:

1. C.C. Pye, T. Ziegler, E. van Lenthe, J.N. Louwen, *An implementation of the conductor-like screening model of solvation within the Amsterdam density functional package. Part II. COSMO for real solvents.* Can. J. Chem. **87**, 790 (2009)

2. ADF2009.01 COSMO-RS, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com
Optionally, you may add the following list of authors and contributors:
J.N. Louwen, C.C. Pye, E. van Lenthe

ADF-GUI and BAND-GUI

The ADF-GUI and BAND-GUI have been developed within SCM (with O. Visser as primary developer).
Main contributions outside SCM have come from:
P. Leyronnas, W.-J. van Zeist, and M. Luppi.

If you used the ADF-GUI (for example ADFview) you may optionally include the reference:

ADF-GUI 2009.01, SCM, Amsterdam, The Netherlands, http://www.scm.com

Likewise if you used the BAND-GUI you may optionally include the reference:

BAND-GUI 2009.01, SCM, Amsterdam, The Netherlands, http://www.scm.com

Feature References ADF

When you have used special features, you should include one (or more, as the case may be) lead reference(s) to the implementation. Additional references to related publications are suggested.

Coordinates, basis sets, fragments

Basis Sets

E. van Lenthe and E.J. Baerends, *Optimized Slater-type basis sets for the elements 1-118.* Journal of Computational Chemistry **24**, 1142 (2003)

Nuclear model

spherical Gaussian nuclear charge distribution model

J. Autschbach, *Magnitude of Finite-Nucleus-Size Effects in Relativistic Density Functional Computations of Indirect NMR Nuclear Spin-Spin Coupling Constants.* ChemPhysChem **10**, 2274 (2009)

Geometry optimizations, transition states, and reaction paths

Transition State search

L. Versluis and T. Ziegler, *The determination of Molecular Structure by Density Functional Theory.* Journal of Chemical Physics **88**, 322 (1988)

L. Fan and T. Ziegler, *Nonlocal density functional theory as a practical tool in calculations on transition states and activation energies.* Journal of the American Chemical Society **114**, 10890 (1992)

IRC

L. Deng, T. Ziegler and L. Fan, *A combined density functional and intrinsic reaction coordinate study on the ground state energy surface of H_2CO.* Journal of Chemical Physics **99**, 3823 (1993)

L. Deng and T. Ziegler, *The determination of Intrinsic Reaction Coordinates by density functional theory.* International Journal of Quantum Chemistry **52**, 731 (1994)

Nudged Elastic Band

G. Henkelman, B.P. Uberuaga and H. Jónsson, *A climbing image nudged elastic band method for finding saddle points and minimum energy paths.* Journal of Chemical Physics **113**, 9901 (2000)

Quild

For calculations with the Quild program

M. Swart and F.M. Bickelhaupt, *QUILD: QUantum-regions interconnected by local descriptions.* Journal of Compututational Chemistry **29**, 724 (2007)

DFTB

For calculations with the Density Functional Tight Binding (DFTB) program

1. T. Frauenheim, G. Seifert, M. Elstner, Z. Hajnal, G. Jungnickel, D. Porezag, S. Suhai and R. Scholz, *A Self-Consistent Charge Density-Functional Based Tight-Binding Method for Predictive Materials Simulations in Physics, Chemistry and Biology.* Physica Status Solidi (b) **217**, 41 (2000)

2. ADF2009.01 DFTB, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com
Optionally, you may add the author: D.A. McCormack

DFTB parameter files available in the ADF package

J. Frenzel, A. F. Oliveira N. Jardillier, T. Heine, and G. Seifert, *Semi-relativistic, self-consistent charge Slater-Koster tables for density-functional based tight-binding (DFTB) for materials science simulations*, TU-Dresden 2004-2009.

Model Hamiltonians

Density Functional

OEP

M. Krykunov and T. Ziegler, *On the use of the exact exchange optimized effective potential method for static response properties*, International Journal of Quantum Chemistry **109**, 3246 (2009)

Relativistic Effects

ZORA

Lead references

E. van Lenthe, E.J. Baerends and J.G. Snijders, *Relativistic regular two-component Hamiltonians.* Journal of Chemical Physics **99**, 4597 (1993)

E. van Lenthe, E.J. Baerends and J.G. Snijders, *Relativistic total energy using regular approximations.* Journal of Chemical Physics **101**, 9783 (1994)

E. van Lenthe, A.E. Ehlers and E.J. Baerends, *Geometry optimization in the Zero Order Regular Approximation for relativistic effects.* Journal of Chemical Physics **110**, 8943 (1999)

Suggested related references

E. van Lenthe, J.G. Snijders and E.J. Baerends, *The zero-order regular approximation for relativistic effects: The effect of spin.orbit coupling in closed shell molecules.* Journal of Chemical Physics **105**, 6505 (1996)

E. van Lenthe, R. van Leeuwen, E.J. Baerends and J.G. Snijders, *Relativistic regular two-component Hamiltonians.* International Journal of Quantum Chemistry **57**, 281 (1996)

Pauli

Lead references

J.G. Snijders, E.J. Baerends and P. Ros, *A perturbation theory approach to relativistic calculations. II. Molecules.* Molecular Physics **38**, 1909 (1979)

P.M. Boerrigter, E.J. Baerends and J.G. Snijders, *A relativistic LCAO Hartree-Fock-Slater investigation of the electronic structure of the actinocenes $M(COT)_2$, M=Th, Pa, U, Np and Pu.* Chemical Physics **122**, 357 (1988)

T. Ziegler, V. Tschinke, E.J. Baerends, J.G. Snijders and W. Ravenek, *Calculation of bond energies in compounds of heavy elements by a quasi-relativistic approach.* Journal of Physical Chemistry **93**, 3050 (1989)

Solvents and other environments

COSMO: Conductor like Screening Model

C.C. Pye and T. Ziegler, *An implementation of the conductor-like screening model of solvation within the Amsterdam density functional package.* Theoretical Chemistry Accounts **101**, 396 (1999)

QM/MM: Quantum mechanical and Molecular Mechanics model

Lead

T. K. Woo, L. Cavallo and T. Ziegler, *Implementation of the IMOMM methodology for performing combined QM/MM molecular dynamics simulations and frequency calculations.* Theoretical Chemistry Accounts **100**, 307 (1998)

Suggested

T. K. Woo, S. Patchkovskii, and T. Ziegler, *Atomic Scale Modeling of Polymerization Catalysts.* Computing in Science & Engineering, **2**, 28-37 (2000)

For AddRemove model

M. Swart, *AddRemove: A new link model for use in QM/MM studies.* International Journal of Quantum Chemistry **91**, 177 (2003)

FDE: Frozen Density Embedding

T.A. Wesolowski and A. Warshel, *Frozen Density Functional Approach for ab-initio Calculations of Solvated Molecules.* Journal of Physical Chemistry **97**, 8050 (1993)

J. Neugebauer, C.R. Jacob, T.A. Wesolowski and E.J. Baerends, *An Explicit Quantum Chemical Method for Modeling Large Solvation Shells Applied to Aminocoumarin C151.* Journal of Physical Chemistry A **109**, 7805 (2005)

C.R. Jacob, J. Neugebauer and L. Visscher, *A flexible implementation of frozen-density embedding for use in multilevel simulations.* Journal of Compututational Chemistry **29**, 1011 (2008)

DRF: Discrete Solvent Reaction Field model

L. Jensen, P.T. van Duijnen and J.G. Snijders, *A discrete solvent reaction field model within density functional theory.* Journal of Chemical Physics **118**, 514 (2003)

SCRF: Self-Consistent Reaction Field

J.L. Chen, L. Noodleman, D.A. Case and D. Bashford, *Incorporating solvation effects into density functional electronic structure calculations*, Journal of Physical Chemistry **98**, 11059 (1994)

MM Dispersion: Molecular Mechanics dispersion-corrected functionals

S. Grimme, *Semiempirical GGA-Type Density Functional Constructed with a Long-Range Dispersion Correction.* Journal of Computational Chemistry **27**, 1787 (2006)

old implementation

S. Grimme, *Accurate description of van der Waals complexes by density functional theory including empirical corrections.* Journal of Computational Chemistry **25**, 1463 (2004)

J.-M. Ducéré and L. Cavallo, *Parametrization of an Empirical Correction Term to Density Functional Theory for an Accurate Description of pi-Stacking Interactions in Nucleic Acids.* Journal of Physical Chemistry B **111**, 13124 (2007)
contact: J.M. Ducere, L. Cavallo, University of Salerno, Italy

Molecular properties with ADF

Frequencies, IR Intensities, Raman, VCD

Numerical Differentiation of Gradients

L. Fan and T. Ziegler, *Application of density functional theory to infrared absorption intensity calculations on main group molecules.* Journal of Chemical Physics **96**, 9005 (1992)

L. Fan and T. Ziegler, *Application of density functional theory to infrared absorption intensity calculations on transition-metal carbonyls.* Journal of Physical Chemistry **96**, 6937 (1992)

Analytical Second Derivatives

A. Bérces, R. M. Dickson, L. Fan, H. Jacobsen, D. Swerhone and T. Ziegler, *An implementation of the coupled perturbed Kohn-Sham equations: perturbation due to nuclear displacements.* Computer Physics Communications **100**, 247 (1997)

H. Jacobsen, A. Bérces, D. Swerhone and T. Ziegler, *Analytic second derivatives of molecular energies: a density functional implementation.* Computer Physics Communications **100**, 263 (1997)

S. K. Wolff, *Analytical second derivatives in the Amsterdam density functional package.* International Journal of Quantum Chemistry **104**, 645 (2005)

Mobile Block Hessian (MBH)

Lead

A. Ghysels, D. Van Neck, V. Van Speybroeck, T. Verstraelen and M. Waroquier, *Vibrational Modes in partially optimized molecular systems* Journal of Chemical Physics**126**, 224102 (2007)

Suggested

A. Ghysels, D. Van Neck and M. Waroquier, *Cartesian formulation of the Mobile Block Hessian Approach to vibrational analysis in partially optimized systems* Journal of Chemical Physics**127**, 164108 (2007)

(Resonance) Raman Scattering

Raman scattering

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Application of time-dependent density functional response theory to Raman scattering.* Chemical Physics Letters **259**, 599 (1996)

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Implementation of time-dependent density functional response equations .* Computer Physics Communications **118**, 119 (1999)

Resonance Raman: excited-state finite lifetime

L. Jensen, L. Zhao, J. Autschbach and G.C. Schatz, *Theory and method for calculating resonance Raman scattering from resonance polarizability derivatives*, Journal of Chemical Physics **123**, 174110 (2005)

Resonance Raman: excited-state gradient

J. Neugebauer, E.J. Baerends, E. Efremov, F. Ariese and C. Gooijer, *Combined Theoretical and Experimental Deep-UV Resonance Raman Studies of Substituted Pyrenes.* Journal of Physical Chemistry A **109**, 2100 (2005)

Vibrational Circular Dichroism (VCD)

V.P. Nicu J. Neugebauer S.K. Wolff and E.J. Baerends, *A vibrational circular dichroism implementation within a Slater-type-orbital based density functional framework and its application to hexa- and hepta-helicenes.* Theoretical Chemical Accounts **119**, 245 (2008)

Time-Dependent DFT

For all Time-Dependent DFT features (Excitation Energies, (Hyper) Polarizabilities, Dispersion Coefficients, Raman Scattering, include:

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Implementation of time-dependent density functional response equations .* Computer Physics Communications **118**, 119 (1999)

Excitation Energies and Oscillator Strengths

Lead reference

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Implementation of time-dependent density functional response equations* . Computer Physics Communications **118**, 119 (1999)

Suggested (when ZORA relativistic results are used)

A. Rosa, E.J. Baerends, S.J.A. van Gisbergen, E. van Lenthe, J.A. Groeneveld and J. G. Snijders, *Article Electronic Spectra of $M(CO)_6$ (M = Cr, Mo, W) Revisited by a Relativistic TDDFT Approach.* Journal of the American Chemical Society **121**, 10356 (1999)

Open Shell ground state

F. Wang and T. Ziegler, Mol. Phys.**102**, 2585 (2004)

Spin-flip transitions

F. Wang and T. Ziegler, *Time-dependent density functional theory based on a noncollinear formulation of the exchange-correlation potential.* Journal of Chemical Physics **121**, 12191 (2004)

F. Wang and T. Ziegler, *The performance of time-dependent density functional theory based on a noncollinear exchange-correlation potential in the calculations of excitation energies.* Journal of Chemical Physics **122**, 74109 (2005)

Core excitations

M. Stener, G. Fronzoni and M. de Simone, *Time dependent density functional theory of core electrons excitations.* Chemical Physics Letters **373**, 115 (2003)

Excitations including spin-orbit coupling

F. Wang, T. Ziegler, E. van Lenthe, S.J.A. vand Gisbergen and E.J. Baerends, *The calculation of excitation energies based on the relativistic two-component zeroth-order regular approximation and time-dependent density-functional with full use of symmetry.* Journal of Chemical Physics **122**, 204103 (2005)

Perturbative approach to include spin-orbit coupling

F. Wang and T. Ziegler, *A simplified relativistic time-dependent density-functional theory formalism for the calculations of excitation energies including spin-orbit coupling effect*, Journal of Chemical Physics **123**, 154102 (2005)

Polarizabilities

Lead

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *A Density Functional Theory study of frequency-dependent polarizabilities and van der Waals dispersion coefficients for polyatomic molecules.* Journal of Chemical Physics **103**, 9347 (1995)

Suggested

V.P. Osinga, S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Density functional results for isotropic and anisotropic multipole polarizabilities and C_6, C_7, and C_8 Van der Waals dispersion coefficients for molecules.* Journal of Chemical Physics **106**, 5091 (1997)

Hyperpolarizabilities

Lead

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Calculating frequency-dependent hyperpolarizabilities using time-dependent density functional theory.* Journal of Chemical Physics **109**, 10644 (1998)

Suggested:

S.J.A. van Gisbergen, J.G. Snijders, and E.J. Baerends, *Time-dependent Density Functional Results for the Dynamic Hyperpolarizability of C_{60}.* Physical Review Letters **78**, 3097 (1997)

Dispersion Coefficients

Lead

V.P. Osinga, S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Density functional results for isotropic and anisotropic multipole polarizabilities and C_6, C_7, and C_8 Van der Waals dispersion coefficients for molecules.* Journal of Chemical Physics **106**, 5091 (1997)

Suggested

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *A Density Functional Theory study of frequency-dependent polarizabilities and van der Waals dispersion coefficients for polyatomic molecules.* Journal of Chemical Physics **103**, 9347 (1995)

Circular Dichroism (CD)

Lead

J. Autschbach and T. Ziegler, *Calculating molecular electric and magnetic properties from time-dependent density functional response theory.* Journal of Chemical Physics **116**, 891 (2002)

J. Autschbach, T. Ziegler, S.J.A. van Gisbergen and E.J. Baerends, *Chiroptical properties from time-dependent density functional theory. I. Circular dichroism spectra of organic molecules.* Journal of Chemical Physics **116**, 6930 (2002)

Optical Rotation (OR), Optical Rotation Dispersion (ORD)

Lead

J. Autschbach and T. Ziegler, *Calculating molecular electric and magnetic properties from time-dependent density functional response theory.* Journal of Chemical Physics **116**, 891 (2002)

J. Autschbach, S. Patchkovskii, T. Ziegler, S.J.A. van Gisbergen and E.J. Baerends, *Chiroptical properties from time-dependent density functional theory. II. Optical rotations of small to medium sized organic molecules.* Journal of Chemical Physics **117**, 581 (2002)

Magnetizability

Lead

M. Krykunov and J. Autschbach, *Calculation of static and dynamic linear magnetic response in approximate time-dependent density functional theory.* Journal of Chemical Physics **126**, 24101 (2007)

Magnetic Circular Dichroism (MCD)

M. Seth, M. Krykunov, T. Ziegler, J. Autschbach and A. Banerjee, *Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism: Calculation of B terms*, Journal of Chemical Physics **128**, 144105 (2008)

M. Seth, M. Krykunov, T. Ziegler and J. Autschbach, *Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism. II. Calculation of A terms*, Journal of Chemical Physics **128**, 234102 (2008)

M. Seth, T. Ziegler and J. Autschbach, *Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism. III. Temperature-dependent magnetic circular dichroism induced by spin-orbit coupling*, Journal of Chemical Physics **129**, 104105 (2008)

Verdet constant and Faraday term

M. Krykunov, M. Seth, T. Ziegler and J. Autschbach, *Calculation of the magnetic circular dichroism B term from the imaginary part of the Verdet constant using damped time-dependent density functional theory*, Journal of Chemical Physics **127**, 244102 (2007)

NMR

NMR Chemical Shifts

Lead reference

G. Schreckenbach and T. Ziegler, *The calculation of NMR shielding tensors using GIAO's and modern density functional theory.* Journal of Physical Chemistry **99**, 606 (1995)

NMR chemical shifts with hybrid functionals

M. Krykunov, T. Ziegler and E. van Lenthe, *Hybrid density functional calculations of nuclear magnetic shieldings using Slater-type orbitals and the zeroth-order regular approximation.* International Journal of Quantum Chemistry **109**, 1676 (2009)

Suggested

G. Schreckenbach and T. Ziegler, *The calculation of NMR shielding tensors based on density functional theory and the frozen-core approximation.* International Journal of Quantum Chemistry **60**, 753 (1996)

G. Schreckenbach and T. Ziegler, *Calculation of NMR shielding tensors based on density functional theory and a scalar relativistic Pauli-type Hamiltonian. The application to transition metal complexes.* International Journal of Quantum Chemistry **61**, 899 (1997)

S.K. Wolff and T. Ziegler, *Calculation of DFT-GIAO NMR shifts with inclusion of spin-orbit coupling.* Journal of Chemical Physics **109**, 895 (1998)

S.K. Wolff, T. Ziegler, E. van Lenthe and E.J. Baerends, *Density functional calculations of nuclear magnetic shieldings using the zeroth-order regular approximation (ZORA) for relativistic effects: ZORA nuclear magnetic resonance.* Journal of Chemical Physics **110**, 7689 (1999)

NMR spin-spin coupling

Lead

J. Autschbach and T. Ziegler, *Nuclear spin-spin coupling constants from regular approximate density functional calculations. I. Formalism and scalar relativistic results for heavy metal compounds.* Journal of Chemical Physics **113**, 936 (2000)

J. Autschbach, and T. Ziegler, *Nuclear spin-spin coupling constants from regular approximate relativistic density functional calculations. II. Spin-orbit coupling effects and anisotropies.* Journal of Chemical Physics **113**, 9410 (2000)

NMR spin-spin couplings with PBE0

J. Autschbach, *Two-component relativistic hybrid density functional computations of nuclear spin-spin coupling tensors using Slater-type basis sets and density-fitting techniques.* Journal of Chemical Physics **129**, 094105 (2008), Erratum: Journal of Chemical Physics **130**, 209901 (2009)

Suggested

R.M. Dickson and T. Ziegler, *NMR Spin.Spin Coupling Constants from Density Functional Theory with Slater-Type Basis Functions.* Journal of Physical Chemistry **100**, 5286 (1996)

J. Khandogin and T. Ziegler, *A density functional study of nuclear magnetic resonance spin.spin coupling constants in transition-metal systems.* Spectrochimica Acta **55**, 607 (1999)

J. Autschbach and T. Ziegler, *Solvent Effects on Heavy Atom Nuclear Spin.Spin Coupling Constants: A Theoretical Study of Hg.C and Pt.P Couplings.* Journal of the American Chemical Society **123**, 3341 (2001)

J. Autschbach and T. Ziegler, *A Theoretical Investigation of the Remarkable Nuclear Spin.Spin Coupling Pattern in $[(NC)_5Pt\text{-}Tl(CN)]^-$.* Journal of the American Chemical Society **123**, 5320 (2001)

Suggested book reference

J. Autschbach, T. Ziegler, in *Encyclopedia of Nuclear Magnetic Resonance*, Eds. D.M. Grant, R. K. Harris, John Wiley and Sons, Chichester, 2002, Vol. 9 *Advances in NMR*.

ESR/EPR

G-tensor: Zeeman interaction

Lead references (EPR/NMR program)

G. Schreckenbach and T. Ziegler, *Calculation of the G-tensor of electron paramagnetic resonance spectroscopy using Gauge-Including Atomic Orbitals and Density Functional Theory.* Journal of Physical Chemistry A **101**, 3388 (1997) (for ESR/EPR g-tensor)

S. Patchkovskii and T. Ziegler, *Calculation of the EPR g-Tensors of High-Spin Radicals with Density Functional Theory*. Journal of Physical Chemistry A **105**, 5490 (2001) (for high-spin ESR/EPR g-tensor)

Lead reference (ADF)

E. van Lenthe, A. van der Avoird and P.E.S. Wormer, *Density functional calculations of molecular g-tensors in the zero order regular approximation for relativistic effects.* Journal of Chemical Physics **107**, 2488 (1997)

A-tensor: Nuclear magnetic dipole hyperfine interaction

Lead reference

E. van Lenthe, A. van der Avoird and P.E.S. Wormer, *Density functional calculations of molecular hyperfine interactions in the zero order regular approximation for relativistic effects.* Journal of Chemical Physics **108**, 4783 (1998)

Electric Field Gradient, NQCC

Lead reference (in ESR called Q-tensor: Nuclear electric quadrupole hyperfine interaction)

E. van Lenthe and E.J. Baerends, *Density functional calculations of nuclear quadrupole coupling constants in the zero-order regular approximation for relativistic effects.* Journal of Chemical Physics **112**, 8279 (2000)

Analysis

Bond Energy Analysis

T. Ziegler and A. Rauk, *A theoretical study of the ethylene-metal bond in complexes between Cu^+, Ag^+, Au^+, Pt^0 or Pt^{2+} and ethylene, based on the Hartree-Fock-Slater transition-state method.* Inorganic Chemistry **18**, 1558 (1979)

T. Ziegler and A. Rauk, *Carbon monoxide, carbon monosulfide, molecular nitrogen, phosphorus trifluoride, and methyl isocyanide as sigma donors and pi acceptors. A theoretical study by the Hartree-Fock-Slater transition-state method.* Inorganic Chemistry **18**, 1755 (1979)

F.M. Bickelhaupt and E.J. Baerends, In: Rev. Comput. Chem.; K.B. Lipkowitz and D.B. Boyd, Eds.; Wiley, New York, 2000, Vol. 15, p.1-86

ETS-NOCV

M. Mitoraj, A. Michalak and T. Ziegler, *A Combined Charge and Energy Decomposition Scheme for Bond Analysis*, Journal of Chemical Theory and Computation **5**, 962 (2009)

Feature References BAND

Lead

See key references above, for all work with BAND

Suggested

G. Wiesenekker, G. te Velde and E.J. Baerends, *Analytic quadratic integration over the two-dimensional Brillouin zone.* Journal of Physics C: Solid State Physics **21**, 4263 (1988)

G. te Velde and E.J. Baerends, *Numerical integration for polyatomic systems.* Journal of Computational Physics **99**, 84 (1992)

Geometry optimization

Lead

E.S. Kadantsev, R. Klooster. P.L. de Boeij and T. Ziegler, *The Formulation and Implementation of Analytic Energy Gradients for Periodic Density Functional Calculations with STO/NAO Bloch Basis Set.* Molecular Physics **105**, 2583 (2007)

TDDFT

Lead

F. Kootstra, P.L. de Boeij and J.G. Snijders, *Efficient real-space approach to time-dependent density functional theory for the dielectric response of nonmetallic crystals.* Journal of Chemical Physics **112**, 6517 (2000)

P. Romaniello and P.L. de Boeij, *Time-dependent current-density-functional theory for the metallic response of solids.* Physical Review B **71**, 155108 (2005)

Main applications

F. Kootstra, P.L. de Boeij, and J.G. Snijders, *Application of time-dependent density-functional theory to the dielectric function of various nonmetallic crystals.* Physical Review B **62**, 7071 (2000)

P. Romaniello, P.L. de Boeij, F. Carbone, and D. van der Marel, *Optical properties of bcc transition metals in the range 0.40 eV.* Physical Review B **73**, 075115 (2006)

Suggested book references

F. Kootstra, Ph.D. thesis, Rijksuniversiteit Groningen, Groningen (2001).

P. Romaniello, Ph.D. thesis, Rijksuniversiteit Groningen, Groningen (2006).

A. Berger, Ph.D. thesis, Rijksuniversiteit Groningen, Groningen (2006).

Relativistic TDDFT

P. Romaniello and P.L. de Boeij, *Relativistic two-component formulation of time-dependent current-density functional theory: Application to the linear response of solids.* Journal of Chemical Physics **127**, 174111 (2007)

Vignale Kohn

Lead

J.A. Berger, P.L. de Boeij and R. van Leeuwen, *Analysis of the viscoelastic coefficients in the Vignale-Kohn functional: The cases of one- and three-dimensional polyacetylene.* Physical Review B **71**, 155104 (2005)

Applications

J.A. Berger, P. Romaniello, R. van Leeuwen and P.L. de Boeij, *Performance of the Vignale-Kohn functional in the linear response of metals.* Physical Review B **74**, 245117 (2006)

J.A. Berger, P.L. de Boeij, and R. van Leeuwen, *Analysis of the Vignale-Kohn current functional in the calculation of the optical spectra of semiconductors.* Physical Review B **75**, 35116 (2007)

External programs and Libraries used by ADF

The next programs and/or libraries are used in the ADF package. On some platforms optimized libraries have been used and/or vendor specific MPI implementations.

Blas: http://www.netlib.org/blas/

Lapack: http://www.netlib.org/lapack/

Scalapack: http://www.netlib.org/scalapack/

Tcl/Tk: http://www.tcl.tk/

Tcllib: http://sourceforge.net/projects/tcllib/

The visualization toolkit (VTK): http://www.vtk.org/

Python: http://www.python.org/

Open Babel: http://openbabel.org/

Symmol: T. Pilati and A. Forni, *SYMMOL: a program to find the maximum symmetry group in an atom cluster, given a prefixed tolerance*, Journal of Applied Crystallography **31**, 503 (1998)

Macroscopic Electrostatics with Atomic Detail (MEAD): http://www.stjuderesearch.org/bashford-mead

Platform MPI 7 (formerly HP-MPI): http://www.platform.com/Products/platform-mpi

Open MPI: http://www.open-mpi.org/